

ENERGY METASTABLE OXYGEN AND NITROGEN ATMOS IN THE TERRESTRIAL ATMOSPHERE

NASA Grant: NAG5-11857

Final Report

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Co-Investigator: A. Dalgarno

Project description

This report summarizes our research performed under NASA Grant NAG5-11857. The three-year grant have been supported by the Geospace Sciences SR&T program. We have investigated the energetic metastable oxygen and nitrogen atoms in the terrestrial stratosphere, mesosphere and thermosphere. Hot atoms in the atmosphere are produced by solar radiation, the solar wind and various ionic reactions. Nascent hot atoms arise in ground and excited electronic states, and their translational energies are larger by two - three orders of magnitude than the thermal energies of the ambient gas. The relaxation kinetics of hot atoms determines the rate of atmospheric heating, the intensities of aeronomic reactions, and the rate of atom escape from the planet. Modeling of the non-Maxwellian energy distributions of metastable oxygen and nitrogen atoms have been focused on the determination of their impact on the energetics and chemistry of the terrestrial atmosphere between 25 and 250 km . At this altitudes, we have calculated the energy distribution functions of metastable O and N atoms and computed non-equilibrium rates of important aeronomic reactions, such as destruction of the water molecules by O(¹D) atoms and production of highly excited nitric oxide molecules. In the upper atmosphere, the metastable O(¹D) and N(²D) play important role in formation of the upward atomic fluxes. We have computed the upward fluxes of the metastable and ground state oxygen atoms in the upper atmosphere above 250 km. The accurate distributions of the metastable atoms have been evaluated for the day and night-time conditions.

Research method

We have analyzed the impact of hot atoms on the atmospheric energy balance, chemistry and excitation of the ro-vibrational motion of the molecules of the ambient gas by solving the time-dependent and steady state Boltzmann kinetic equation with accurate

cross sections for the elastic, inelastic and reactive atmospheric collisions. The kinetics of the metastable atoms, the intensities of their reactions and upward fluxes are very sensitive to the differential cross sections, describing angular distribution of scattering particles at different energies. Our calculations have been carried out with accurate differential cross sections, derived from quantal and semiclassical calculations of collisions between hot and thermal atoms and molecules.

Results.

Results of our investigations of the hot metastable atoms in the terrestrial atmosphere have been published and reported on AGU Meetings:

- Kharchenko, V., A. Dalgarno, and J. L. Fox, *Fast $O(^1D)$ atoms in the thermosphere*, *J. Geophys. Res.*, to be submitted, April, (2005).
- Kharchenko, V. and A. Dalgarno, *Thermalization of fast $O(^1D)$ atoms in the stratosphere and mesosphere*, *J. Geophys. Res.*, **109**, D18311 (2004)
- V. Kharchenko and A. Dalgarno "Hot $O(^1D)$ atoms in the stratosphere and mesosphere", *EOS Trans. AGU*, **85**, JA351 (2004)
- V. Kharchenko and A. Dalgarno "Diurnal variations of energetic $O(^3P)$ and $O(^1D)$ atoms in the thermosphere and mesosphere", *EOS Trans. AGU*, **83**, F1106 (2002)
- V. Kharchenko and A. Dalgarno "Distribution of energetic $O(^3P)$ and $O(^1D)$ atoms in the lower thermosphere and mesosphere", *EOS Trans. AGU*, **83**, S236 (2002)

New results for the stratosphere and mesosphere:

- The thermalization of metastable oxygen atoms in the stratosphere and mesosphere has been investigated. Non-Maxwellian $O(^1D)$ distributions have been calculated at altitudes of 25 and 50 km taking into account the energy-transfer and quenching collisions of fast $O(^1D)$ atoms with the ambient gas. The evolution of the energy distributions of nascent metastable oxygen atoms, produced by ozone photolysis, has been determined by solving the time-dependent Boltzmann equation.

- The time-dependent and steady state $O(^1D)$ distributions have been computed and used for calculations of the parameters, characterizing $O(^1D)$ thermalization and quenching in the stratosphere and mesosphere.
- The steady state $O(^1D)$ distributions contain 3 - 5% of non-thermal atoms, fractions which are significantly larger than those of non-thermal ground state oxygen or nitrogen atoms. The effective temperature of the non-Maxwellian distributions have been found to be 14% and 33% higher than thermal temperatures of the ambient gas at 25 and 50 km.
- The non-equilibrium rate coefficients and yields of NO molecules in the atmospheric reaction $O(^1D) + N_2O$, corresponding to the non-Maxwellian distributions of $O(^1D)$ atoms, have been calculated at the altitudes between 25 and 50km.

New results for the thermosphere:

- Detailed calculations are carried out of the sources of energetic metastable $O(^1D)$ atoms in the atmosphere at altitudes between 80 km and 250km and the corresponding energy distribution functions are derived, taking account of energy transfer and quenching in collisions of the metastable atoms with the ambient atmospheric gas constituents.
- The energy relaxation of metastable oxygen atoms produced by O_2 and O_3 photolysis and O_2^+ dissociative recombination is determined by solving the time-dependent Boltzmann equation. The $O(^1D)$ thermalization and quenching times are obtained as functions of the altitude.
- The steady state and time-dependent distributions of metastable $O(^1D)$ are computed and used for the determination of the parameters characterizing the non-thermal $O(^1D)$ atoms. The non-thermal atoms comprise 4 - 6% of the distribution, and their effective temperatures are larger by 25% - 46% than the local temperatures of the ambient gas.
- The role of hot metastable oxygen atoms in the production of vibrationally excited OH molecules is analyzed.

Table 1: Parameters of hot O(¹D) atoms for the daytime atmosphere.

Altitude [km]	Thermalization time τ_{th} [s]	Quenching time τ_q [s]	Hot O(¹ D) Fraction ξ [%]	T_{eff}/T [%]	O(¹ D) Density 10^3cm^{-3}
80	$1.1 \cdot 10^{-4}$	$1.5 \cdot 10^{-3}$	5	138	0.24
100	$2.6 \cdot 10^{-3}$	0.035	4.3	146	8.2
120	0.047	0.6	4.9	133	18.3
140	0.17	2.18	4.7	125	9.5
160	0.39	4.9	4.8	129	8.0
180	1.0	8.4	5.1	132	7.7
200	1.1	13.5	5.5	137	8.9

In Fig.1 the results of our calculations of the distribution functions of the metastable O(¹D) atoms in the stratosphere, mesosphere, and thermosphere are shown.

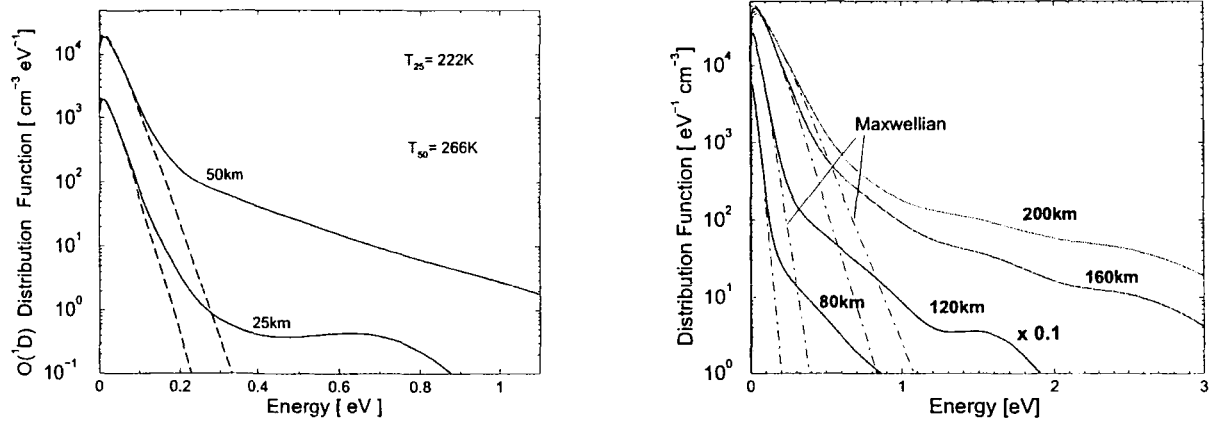


Fig.1 (a) The steady state distributions of metastable O(¹D) atoms at 25 and 50 km. The Maxwellian distributions at 25 and 50 km are given by dashed-dot curves. The solar zenith angle is 30°, and the latitude is 30°N. **(b)** The noon distribution functions between 80 and 200 km. The value of the distribution function at 120 km have been reduced by 10 for convenience in plotting.

The parameters of the hot metastable atoms are given in the Table.